# Combining Bayesian Optimization and Neural Network to Optimize the Plasma Wakefield Acceleration

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The computational cost of finding the optimal design of plasma wakefield acceleration (PWFA) is usually very demanding due to many variables involved. Herein, we have developed a novel framework which combines Bayesian Optimization (BO) with neural network (NN), to replace computationally expensive simulation software and provide a more efficient way for the optimization process. In order to verify this framework, the AWAKE Run 2 experiment at CERN is used as an example. In the framework we constructed, the coefficients of determination  $(R^2)$  of NN reaches above 0.99, and the time-to-solution reduces to a factor of 35.6. For the first time, BO combined with NN is successfully applied to optimize PWFA and significant improvements have been demonstrated. The framework established here in principle can also be extended to the optimization of other particle accelerations.

Keywords: Plasma wakefield acceleration, Bayesian optimization, Neural network

### I. INTRODUCTION

For traditional radio-frequency (RF) based accelerators, it 3 is preferable to increase the feed-in power of the RF cavity increase the acceleration gradient. However, a continu-5 ous increase of the cavity voltage will lead to the electrical 6 breakdown of cavity materials, which poses a fundamental 7 limit for conventional accelerators. On the other hand, the 8 plasma-based accelerators, either driven by a ultrashort and 9 intense laser pulse or a relativistic particle bunch, can sus-10 tain GV/cm acceleration gradient[1-3], i.e. more than three 11 orders of magnitude compared with the conventional accel-12 erators. Therefore, the plasma-based accelerators can greatly 13 reduce the footprint of future accelerators and their associ-14 ated construction and operation cost. It is envisaged that the 15 plasma-based accelerators will find many applications in pro-16 viding high quality particle beams for free electron lasers [4– 17 7], fixed target experiments and energy frontier colliders [8– 11]. 18

In the process of design and optimization of a plasma ac-20 celerator, many variables, including plasma parameters, driv-21 ing beam parameters and witness parameters should be taken 22 into account simultaneously. To obtain a high quality beam, 23 it is often necessary to continuously optimize these variables, <sup>24</sup> such as brute force search or use of optimization algorithms. 25 Brute force search requires a lot of computing resources and 26 time, which increases exponentially with the number of vari-27 ables [12]. Once the number of variables is too large, the calculation time required will be unacceptable. The use of optimization algorithms, such as genetic algorithm [13, 14], particle swarm optimization algorithm [15] and Bayesian Optimization (BO) algorithm [16, 17], can reduce the time to find

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32 the optimal solution to a certain extent [18]. But if there are 33 multiple optimization problems in the same variable range, 34 the algorithm optimization process needs to be repeated for each optimization problem, which also brings an increase in time and computing resources. The neural network(NN), however, can solve this problem very well. The training set data is generated through the simulation software. The model generated by the NN training can be used to replace the simu-40 lation software for prediction when the prediction accuracy is 41 sufficient. When there are multiple variables, it is no longer <sup>42</sup> necessary to use simulation software to calculate, and the re-43 sults can be predicted through the trained neural NN instead.

BO is an efficient machine learning tool for solving multi-45 variable, complex objective functions [16, 17]. It has been 46 successfully applied to several laser-driven electron accelera-47 tion simulations [19, 20] and experiments [21, 22]. The cal-48 culation of the objective function value in the BO process is often obtained through simulation data from software or data 50 collected from experiments, which requires a lot of computing resources and time. In this paper, in the calculation of 52 the objective function value in the BO process, the predicted value from the NN is used instead of the calculated value of the simulation software. Since the prediction time using the NN is much less than the calculation time using simulation software, this greatly reduces the calculation time and computing resource requirement. In addition, when different physical problems need to be optimized simultaneously, the use of NN predictions can greatly reduce the computing resources [23]. In this paper, we introduce this novel framework that combines BO and NN, by taking AWAKE Run 2 experiment at CERN as an example, to demonstrate the effectiveness of this method. Section II introduce the physical 64 problems of AWAKE Run 2 and methods used. Work flow 65 and optimization results are given in Section III and IV. The 66 discussion and conclusion are presented in Sections V and VI, 67 respectively.

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### II. METHODS

#### Physical problems and parameter settings in AWAKE

The Advanced WAKEfield (AWAKE) experiment at CERN is the world first and only proton-driven plasma wake-72 field acceleration (PWFA) experiment [24-27]. The first phase of AWAKE experiment (2016-2018) has successfully demonstrated the self-modulation of a long proton bunch <sub>75</sub> and acceleration of an externally injected low energy (~18.5 76 MeV) electron bunch up to 2 GeV in a single stage of 10 m 77 long plasma channel [37–39]. The current experiment, so- 118 six variables are shown in Table 1, and the witness bunch po-80 ficiently low emittance for high-energy physics applications 122 wakefield. 81 [8, 9].

The AWAKE Run 2 experiment uses the CERN SPS 400 83 GeV proton beam with an RMS length of 6-12 cm, after self-84 modulation in a plasma [29-31], multiple micro-bunches are 85 formed as the driving beam for the PWFA [32]. In the previ-86 ous study, the toy model [33] is used to adjust the charge of 87 the proton beam to make the plasma wakefield reach the de-88 sired acceleration gradient. The proton beam energy, bunch 89 length and beam radius are 400 GeV, 40  $\mu$ m, and 200  $\mu$ m, 90 respectively. In addition, the mismatch of the beam radius on lead to a significant beam emittance growth [33, 40]. The 92 matched radial beam size for a Gaussian beam in the plasma 93 ion column is defined by [33, 41]:

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$$\sigma_r = \left(\frac{2\varepsilon_0}{\gamma_0 k_n^2}\right)^{\frac{1}{4}},\tag{1}$$

where  $k_p = \frac{\omega_p}{c}$  is the plasma wave number,  $\varepsilon_0$  is the initial ge-96 ometric emittance,  $\gamma_0$  is the initial mean Lorentz factor,  $\omega_p$  $_{
m 97}$  and c are the plasma oscillation frequency and the speed of  $_{98}$  light, respectively.  $\omega_p$  is determined by the plasma density  $n_0$ 99 and is given by

$$\omega_p = \sqrt{\frac{n_0 e^2}{m_e \epsilon_0}},\tag{2}$$

where  $e, m_e$  and  $\epsilon_0$  are the electron charge, electron mass and 102 the permittivity of free space, respectively. According to Eqs. (1) and (2), the calculated plasma density is  $7 \times 10^{14}$  cm<sup>-3</sup>. Fig. 1 gives the schematic diagram of AWAKE Run 2 setup. It uses a 400 GeV proton beam to pass through a 10 105 m long plasma to excite the wakefield. The electron beam is injected externally, and the appropriate acceleration phase is set by adjusting the position between the driving beam and the witness bunch. The electrons will be captured by the plasma wakefield and accelerated. In the simulation of AWAKE Run 2 experiment, the toy model is employed. The parameters of the driving bunch and the plasma are fixed and the initial energy of the witness bunch is set to 150 MeV [28, 34]. The optimal solution is obtained by optimizing the acceleration 155 115 distance and five parameters of the witness bunch, i.e., the 156 tion. It will predict the probability of the target value correbunch charge, bunch length, emittance, energy spread and its 157 sponding to the variable space based on the data of all pre-

TABLE 1. Variables in the optimization problem and the corresponding range of variation

Variables	Variation range
Acceleration distance	0 - 10 m
Witness bunch charge	50 - 300 pC
Witness bunch length	$40$ - $120~\mu\mathrm{m}$
Witness bunch emittance	4 - 10 mm·mrad
Witness bunch position	$5.8 - 6.7 k_p^{-1}$
Witness bunch energy spread	0.1% - 0.5%

78 called AWAKE Run 2 [28], aims to accelerate an electron 119 sition is the distance between the witness bunch and the driv-<sub>79</sub> bunch up to  $\sim 10$  GeV with a narrow energy spread and suf-<sub>120</sub> ing bunch, in  $k_p^{-1}$ .  $2\pi/k_p$  is the wavelength of the plasma

#### Neural Network

In a fully connected NN, each neuron is connected to all neurons in the previous layer, so a weight matrix is needed to 126 describe these connections. This weight matrix is called the 127 kernel, which determines how the output of neurons in the 128 previous layer is combined into the input of the neurons of 129 the current layer. In addition, each neuron also has a learnable bias parameter, which is a constant added to the input of all neurons in the current layer to adjust the output of the model. 132 The output of the neuron is activated only when the input to 133 the neuron exceeds a certain threshold, which is controlled by (1) 134 a bias parameter. As shown in Fig. 2, each network layer contains kernel and bias parameters. During the training process, the network will automatically learn these parameters so that the prediction results of the model are as close as possible to the true value. The goal of optimization is to obtain the best 139 beam quality, including witness bunch energy, energy spread, 140 emittance and charge after being accelerated in plasma wake-141 field in a 10-meter-long plasma. Therefore, when training 142 the NN for this physics problem, the NN should contain one (2) 143 input layer with six neurons and one output layer with four 144 neurons. After optimization, the number of hidden layers of 145 the NN is set to four, and each hidden layer contains 100 neu-146 rons. Within the range of variables, 2000 variable combi-147 nations were randomly sampled, and the corresponding four 148 parameters of the witness bunch after 10-meter acceleration are calculated by the simulation software LCODE [35, 36]. 150 The 2000 events obtained from LCODE simulation are used 151 to train the NN, of which 1600 events are used as the training set, 200 events are used as the verification set, and the 153 remaining 200 events are used as the test set.

# BO algorithm

BO is an efficient algorithm for finding the optimal soluposition from the driving bunch. The variation ranges of the 158 vious iterations, then select the variable corresponding to the

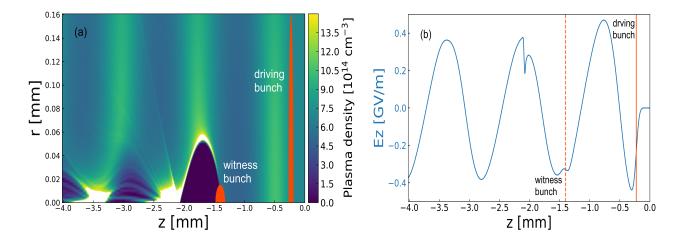


Fig. 1. Schematic diagram of proton beam driven plasma wakefield acceleration. (a) The plasma charge density distribution during the PWFA process. The black part is the bubble region generated by the proton beam driving the plasma wakefield. The left and right orange parts are the relative positions of the witness bunch and the driving bunch in the plasma, respectively. (b) The blue curve is the electric field distribution of the plasma wakefield. The orange dashed and solid lines show the relative positions of the witness bunch and the driving bunch in the plasma wakefield, respectively.

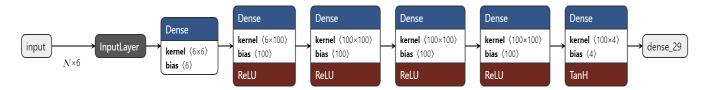


Fig. 2. Schematic diagram of a fully connected NN. The figure shows the dimensions of the internal kernel and bias matrix of the NN. The hidden layer uses the Rectified Linear Unit (ReLU) activation function, and the output layer uses the Hyperbolic Tangent (TanH) activation function, which maps the input of the neuron to the output. " $N \times 6$ " indicates the dimension of the input tensor. "N" is the number of samples in the data set, indicating the uncertainty of a certain dimension, which allows the NN to accept any number of samples as input and adapt to different input data set sizes. "6" is the number of eigenvalues for each sample, which is the 6 variables mentioned above.

159 predicted optimal target value as the next generation, and con- 175 tinuously get a better solution. In the AWAKE Run 2 optimization problem, J. P. Farmer and L. Liang et al. develop a single figure of merit that can give rise to constraints on both the tunability and stability of the initial witness bunch parameters [40]. After the NN is trained, the BO combined with NN framework can be used to optimize according to different optimization objectives. Here we take a four-dimensional target as an example, including the energy (E), energy spread  $(\delta)$ , emittance  $(\varepsilon)$  and charge (Q) of the electron bunch. There-168 fore, when using BO, the f value of Eq. (3) is used as the single-objective optimization. The larger the f, the better the beam quality. In this BO combined with NN framework, different optimization objectives can be selected according to different research problems.

$$f = \frac{E(GeV) \cdot Q(pC)}{\delta(\%) \cdot \varepsilon(mm \cdot mrad)}.$$
 (3)

# III. WORK FLOW

As shown in Fig. 3, we first use the plasma wakefield simulation software LCODE to randomly generate 2000 events as data set, and then randomly divide the data set into training set, verification set and test set according to the ratio of 8:1:1. We then build a fully connected NN with 6 inputs and 4 outputs. Through inputting the training set and verification set data into the NN, we can continuously adjust the NN parameters, including the number of hidden layers, learning rate, batch size and the number of neurons in the hidden layer. Finally, the parameters combination with the highest prediction accuracy of the test set data are selected as the trained NN.

After the NN is trained, the BO algorithm is used to optimize the problem. During the optimization process, when
the initial sampling point is generated and the goal value of
the new observation point is calculated, the objectives value
predicted by the NN is used to calculate the goal value. For
different optimization objectives, the convergence iterations
of the optimization process is also different. In order to ensure the convergence of BO, a higher iteration threshold for
the end of BO is set in the workflow. When the number of

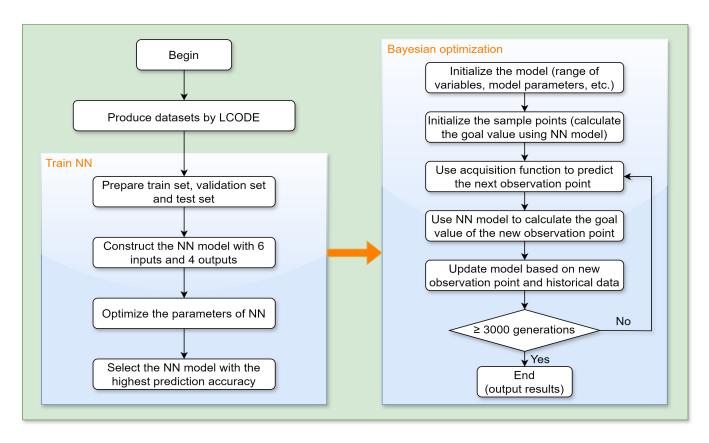


Fig. 3. Optimizing proton-driven PWFA using BO with NN. The blue area on the left is the training NN workflow, and the blue area on the right is the BO process.

196 iterations reaches 3000, the optimization iteration ends, and 197 the optimal solution parameters and goal values are output.

# IV. RESULTS

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## Training Neural Network

By optimizing the parameters of the NN including the 200 201 number of hidden layers, learning rate, number of neurons 202 and epoch, a feed-forward NN for the AWAKE Run 2 prob- $_{
m 203}$  lem is established. Suppose a data set includes a total of  $y_1$  $y_n$  observations, and the corresponding model predicted values are  $f_1$  to fin respectively. The coefficients of determi-206 nation  $(R^2)$  is calculated by the following:

$$R^{2} = 1 - \frac{\sum_{i=1}^{n} (y_{i} - f_{i})^{2}}{\sum_{i=1}^{n} (y_{i} - \bar{y})^{2}}, \ \bar{y} = \frac{1}{n} \sum_{i=1}^{n} y_{i}.$$
 (4)

predicted by the NN in the calculation test set and the target  $\frac{228}{10}$  in Fig. 5, after 3000 iterations, the highest f-value is at genvalue calculated by LCODE, is close to 1, indicating that the 229 eration 2860. 212 prediction accuracy is high. The  $R^2$  values of the six objec- 230 The f-value of the 2860<sup>th</sup> generation is the highest, which  $^{213}$  tives are shown in Table 2, and the average  $R^2$  value reaches  $^{231}$  is the optimal solution obtained by the optimization. At 214 0.9975.

TABLE 2.  $R^2$  values for the four objectives in the test set.

			Emittance	Charge	Average
$R^2$ value	0.9999	0.9989	0.9917	0.9996	0.9975

There are 200 events in the test set, and the comparison 216 between the value predicted by the NN and the value calcu-217 lated by LCODE is shown in Fig. 4. The beam energy, en-218 ergy spread, emittance and bunch charge are compared from 219 top to bottom. The blue point is calculated by LCODE and 220 the orange point is predicted by the NN. The pink points are the error values for each individual between calculation and 222 prediction. The closer the prediction is, the better the NN

# BO with NN

We employ the BO to optimize the AWAKE Run 2 prob-Through the evaluation of the  $R^2$  parameter, the accuracy 226 lem, and use the f value as the single-objective optimization. of NN prediction, that is, the  $R^2$  between the target value 227 The larger the f value, the better the beam quality. As shown

232 this time, the corresponding variables, namely the bunch

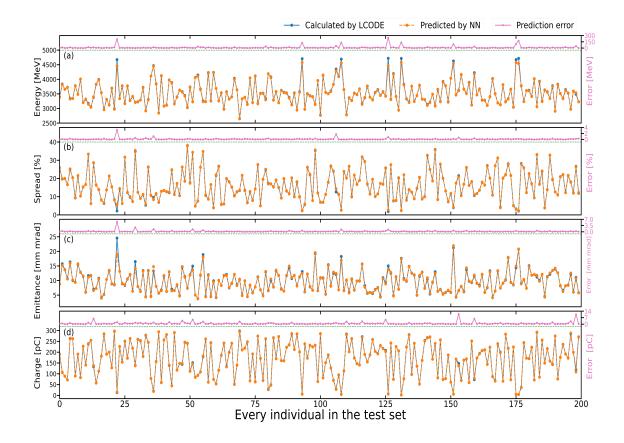


Fig. 4. The comparison between the NN prediction value and the LCODE calculation value of each data individual in the test set containing 200 events. (a), (b), (c) and (d) are the output beam energy, energy spread, emittance and charge respectively. The blue points are the calculated value of LCODE, the orange points are the predicted value of the NN model. The pink points are the error values for each individual between the value predicted by the NN and the value calculated using LCODE.

after a 10 m accelerate distance. The corresponding target 257 optimization problems. values are as shown in Table 3. The first row is the result predicted by the NN, and the second row is calculated by LCODE to verify the accuracy of the prediction. It can be 258 seen that each target value predicted by the NN is close to the result obtained by the LCODE calculation and verification, 259 indicating that the prediction accuracy of the NN is high.

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timal solution, so the convergence trend of each variable can 262 process. Strategy 2 is the approach discussed above, which be judged by the distribution density of the polylines in the 263 uses framework (BO combined with NN) for optimization. parallel axis coordinate graph. As shown in Fig. 6, the denser 264 The advantage of using BO combined with NN compared the polyline is, the more likely it produces a better solution 265 to the approach of BO and simulation software LCODE in find that the energy spread has the highest percentage in the 268 to calculate once, as well as the number of computer cores importance, indicating that the initial energy spread of wit- 269 used by different processes and their corresponding values 252 ness bunch plays a more important role for optimizing the 270 are shown in Table 4. Time-to-solution is the time required goal. This means, in the process of optimization to find the 271 to find the optimal solution. Because the time spent using dif-254 optimal solution, initial energy spread is the main variable, 272 ferent numbers of cores is different, therefore, when calculat-

charge, bunch length, emittance, position and energy spread 255 and changing the initial energy spread has the greatest impact are 135.13 pC, 41.49  $\mu$ m, 2.00 mm·mrad, 5.95 and 0.17% 256 on the goal value, which can provide empirical help for our

# DISCUSSION

Here we compare the time-to-solution and computational 260 resources of the two strategies. Strategy 1 is to use BO, In the BO process, there is a tendency to approach the op- 261 and LCODE is used for calculation during the optimization within this dense range. Through the calculation of hyperpa- 266 terms of time is evaluated from Bellotti's method [23]. The rameter importance in the BO process, as shown in Fig. 7, we 267 time required for different processes such as using LCODE

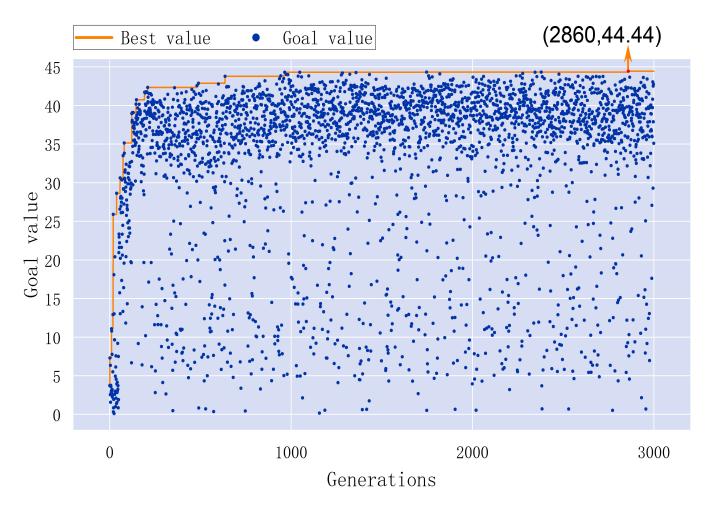


Fig. 5. BO iteration figure. The blue points represent the f-values calculated for each iteration, and the points on the orange line represent that the f-values of each new iteration are higher than the f-values of all previous generations. The red point indicates the highest goal value, that is, the optimal solution, which is the  $2860^{th}$  generation in the optimization process.

TABLE 3. The NN prediction value of the optimal solution and the verification value calculated by LCODE.

	Energy(MeV)	Spread(%)	Emittance(mm·mrad)	Charge(pC)	f-value
NN	3509.85	2.94	3.63	135.34	44.44
LCODE	3529.50	2.91	3.52	135.10	46.55

<sub>273</sub> ing time-to-solution, it is assumed that computing resources <sub>289</sub> 35.59 and  $c_{LCODE}/c_{FW} \approx 1.0$ , respectively, which shows 274 are unlimited, i.e., there are infinite cores that can be used. 290 that the method of using NN instead of simulation software 275 The time  $t_{LCODE}$  required to find the optimal solution us- 291 is more advantageous in terms of time-to-solution. After the 276 ing the strategy of BO with simulation software is shown in 292 NN is trained, different objective functions can be used for 277 Eq. (5). Eq. (6) is the time  $t_{FW}$  to find the optimal solu- 293 optimization according to different research problems. When 278 tion using the framework. The ratio of the two shown in Eq. 294 the number of research problems is greater than 1, the com-282 spectively, considering the number of cores used for LCODE 298 vantage. This is because training the neural network itself re-285 (10) is the ratio of the two, which reflects the comparison 301 lems will not increase the computational cost of training the 286 of the computing resource usage of the two strategies. By 302 NN. If there are more than one research problems, the ad-287 calculating the ratios of the two strategies in terms of time- 303 vantages of combining the optimization algorithm and NN in 288 to-solution and computational cost, they are  $t_{LCODE}/t_{FW} \approx 304$  time-to-solution and computational cost will increase as the

(7) gives the time saved by using the neural NN instead of 295 putational cost of using the framework will exceed 1, indithe simulation software. In addition, the usage of computing 296 cating that when the NN is used at least twice to optimize resources of the two strategies is shown in Eqs.(8) and (9) re- 297 different problems, the computational cost will show an adcalculation and training NN.  $c_{LCODE}$  and  $c_{FW}$  are the com- 299 quires computational costs caused by data set support. After puting resources used by strategies 1 and 2, respectively. Eq. 300 training the NN, the optimization of different research prob-

TABLE 4. Parameters related to the speedup calculation.

Quantity	Symbol	Value
Time for calculating one event by LCODE	$t_0$	2.26 min
Time to train one neural network model	$t_t$	2.77 h
Time to predict once with the framework	$t_p$	0.44 s
Number of event for training NN model	n	2000
Number of hyperparameters to try	$n_h$	120
Number of CPU cores per evaluation by LCODE	$r_0$	72
Number of CPU cores to train and evaluate the framework	$r_t$	8
Number of generations	$n_g$	3000
Number of individuals per generation	$n_i$	1



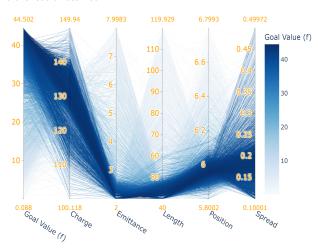


Fig. 6. During the BO process, the line graph of each generation's target f-value and the corresponding variables.

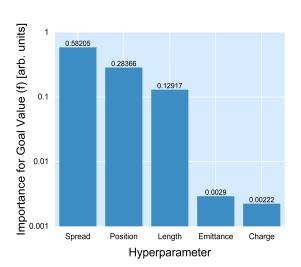
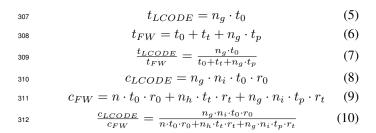


Fig. 7. Hyperparameter importance of BO.

306 number of research problems increases, as shown in Fig. 8.



# VI. CONCLUSION

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Our results have shown that for the AWAKE Run 2 optimization process, the combination of BO and NN can significantly reduce the computing time and the requirement for computing resource usage for finding the optimal solution under a certain computing accuracy. The data calculated by the simulation software LCODE is used as the training set of the NN, and a NN with 6 inputs and 4 outputs has been successfully trained. In the BO process, the prediction ability of the

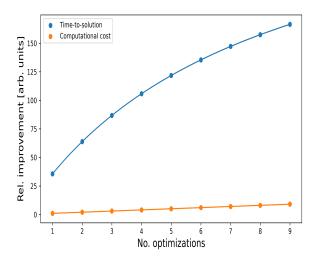


Fig. 8. Relative improvement in terms of time-to-solution and computational cost.

322 NN is used to replace the calculation process of the simula- 336 323 tion software to find the optimal solution of the goal function. 324 The results show that the framework reduces the optimiza-325 tion time (by speedup factor of 35.59), that is, about 35.59 326 times less computational time, which will increase if multi-327 ple optimizations need to be performed, because the training model is the main time-consuming and computationally intensive part. For more complex physical problems with more 339 variables, it will be more advantageous to use NN instead of simulation software in the stage of BO. In this paper, first use 340 of BO combined with NN to optimize PWFA, which demon- 341 nology Project of Hubei Province(2021AFB001). strates the great potential in the optimization of other parti- 342 cle accelerations, especially when the setup involves multiple 343 the supercomputing system in the Supercomputing Center of 335 variables.

# DATA AVAILABILITY STATEMENT

The data that support the findings of this study are available 338 from the corresponding author upon request.

### ACKNOWLEDGMENTS

This work was supported by the Major Science and Tech-

The numerical calculations in this paper have been done on Wuhan University.

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